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METHOD FOR DETERMINING CRYSTALLOGRAPHIC ORIENTATION

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ABSTRACT OF THE DISCLOSURE

Crystal orientation is determined using a single Laue photograph which is employed to determine the orientation of the crystal for scanning on an X-ray diffractometer.

This application is a division of application Ser. No. 455,716 filed May 14, 1965, now abandoned.

My invention relates to a method and apparatus for determining crystal orientation. In particular, it relates to a method and apparatus for determining crystal orientation by means of a diffractometer and a single Laue photograph.

In recent years, the physical and chemical properties of materials have undergone an increasingly detailed investigation. It is well known that the structure of material strongly influences its properties and accordingly the attention of experimental metallurgists has often strongly centered on the determination and classification of the structural properties of a wide variety of materials. Many materials exhibit a regular structure on the atomic level; an example of this is found in crystalline materials, which exhibit an ordered and repeated structure throughout the extent of the crystal. If a suitable reference system is chosen at any point within the crystal, it will be found that the atoms with the structure may be considered to lie in planes which intercept the reference axes at various distances. The magnitude of the intercept of these planes with the reference axes is characteristic of the plane under consideration and serves to identify the plane. For various reasons however, which need not be considered here, it has been found useful to identify the crystal planes by means of the reciprocals of these intercepts; these reciprocals are well known as the Miller indices of the plane. Thus the (224) plane of a crystal may be recognized as that plane which intersects the three reference axes at ½ unit, ½ unit, and ¼ unit from the reference origin respectively. The number and types of planes which a crystal possesses, the spacing between these planes, and the angles which these planes make with the reference axes are important characteristics of the particular crystal under study. The orientation of these planes with respect to the reference axes will hereinafter be referred to as the crystal orientation.

Several techniques have been utilized for determining crystal orientation, most of which are of limited applicability. Thus, for example, the internal structure of a crystal may often be releaved by examination of the external faces of the crystal or by examining the manner in which a crystal may be broken into separate pieces by pressure at various surface points thereof. A more powerful and more nearly exact technique for the determination of crystal orientation, however, lies in the use of X-ray analysis. Since the spacing of the atoms within the crystal structure is of the order of the wave length of X-rays (1–2 angrstroms), crystals which are irradiated with X-rays will diffract these rays in a determinable manner. Indeed it has been found that if a plane of a

crystal is exposed to X-rays, the crystal will diffract these rays at an angle given by $n\lambda - 2d \sin \theta$, where n is any integer and denotes the "order" of diffraction, λ is the wave length of the incident X-rays, d is the spacing between parallel crystal planes (interplanar spacing) and θ is the angle between the incident X-ray and the crystal plane (the angle between the diffracted ray and the crystal plane also equals θ). This relation is known as Bragg's law and the angle θ is known as the Bragg angle. The diffracted rays may be detected and measured by photographic or electronic means to provide an indication of the crystal orientation or may be subjected to X-ray analysis by means of a diffractometer, for example, which consists of a table for mounting a crystal specimen, a source of monochromatic X-rays for irradiating the specimen, and a detector for measuring the orientation and intensity of the diffracted rays.

One well known method for performing the initial orientation of the crystal is to utilize a back reflection Laue photograph technique in which the crystal having planes whose orientation is unknown is irradiated with X-rays and the diffracted rays from the crystal are intercepted by a photographic plate on which the diffracted rays impinge, thereby causing a series of spots to appear on the film. These spots are due to the rays diffracted from various planes within the crystal and the location and spacing of the spots may be used to determine the crystal orientation. In particular, the angular orientation of any one of these spots with respect to the center of the film will define the location of the normal to the plane responsible for the diffraction associated with that spot. The identification of this plane will still be incomplete, however, since the crystallographer must know not only the relative orientation of the plane causing the diffraction (as determined by the Laue photograph) but must also have some knowledge of the interplanar angles or interplanar spacing before Miller indices can be assigned to the planes. The process of determining the orientation of unidentified planes in the crystal will be referred to herein as relative orientation of the crystal, while the process of determining the orientation of unidentified planes and assigning Miller indices to them will be referred to as complete determination of crystal orientation or, more briefly, as critical orientation.

Prior attempts to identify the crystal planes by means of Laue photographs involved either examination of a series of these photographs or, alternatively, determination of the crystal orientation by a series of cut and try steps in which Miller indices were tentatively assigned to a particular diffraction spot (or rather the "pole" of this spot plotted on what is known as a stereographic projection) and the Miller indices of the remaining spots were deduced from this by means of the known interplanar angles and interplanar spacing for a crystal of the class being studied. If the initial assumption were correct, the poles on the stereographic projection would be found to bear the proper indices and the proper relation to neighboring poles required for crystals of that class. Often, however, the initial assumption would be incorrect as revealed by the "identification" of poles which did not belong in the class of crystal under study and the process was repeated as often as necessary with new sets of Miller indices being assigned to the original pole at each repetition. This process could be long and laborious, and often required the services of a skilled crystallographer who could utilize such factors as the presence of symmetry elements to reduce the complexity of the identification process.

Accordingly, it is an object of my invention to provide an improved method for determining the complete orientation of the planes of a crystal. A further object